

Algebraic Aspects of Multiple Zeta Values

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Abstract

Multiple zeta values have been studied by a wide variety of methods. In this article we summarize some of the results about them that can be obtained by an algebraic approach. This involves “coding” the multiple zeta values by monomials in two noncommuting variables x and y . Multiple zeta values can then be thought of as defining a map $\zeta : \mathfrak{H}^0 \rightarrow \mathbf{R}$ from a graded rational vector space \mathfrak{H}^0 generated by the “admissible words” of the noncommutative polynomial algebra $\mathbf{Q}\langle x, y \rangle$. Now \mathfrak{H}^0 admits two (commutative) products making ζ a homomorphism—the shuffle product and the “harmonic” product. The latter makes \mathfrak{H}^0 a subalgebra of the algebra QSym of quasi-symmetric functions. We also discuss some results about multiple zeta values that can be stated in terms of derivations and cyclic derivations of $\mathbf{Q}\langle x, y \rangle$, and we define an action of QSym on $\mathbf{Q}\langle x, y \rangle$ that appears useful. Finally, we apply the algebraic approach to relations of finite partial sums of multiple zeta value series.

1 Introduction

The last fifteen years have seen a great deal of work on the multiple zeta values (MZVs)

$$\zeta(i_1, i_2, \dots, i_k) = \sum_{n_1 > n_2 > \dots > n_k \geq 1} \frac{1}{n_1^{i_1} n_2^{i_2} \dots n_k^{i_k}}, \quad (1)$$

where i_1, i_2, \dots, i_k are positive integers. The case $k = 2$ goes back to Euler [8], and was revisited by Nielsen [28] and Tornheim [35]. The general case was introduced in [17] and [39]. These quantities have appeared in a surprising variety of contexts, including knot theory [25], quantum field theory [4, 24], and even mirror symmetry [20].

Much work on MZVs has focused on discovering and proving identities about them, particularly those that express MZVs of “length” (k in equation (1)) greater than one in terms of ordinary (length one) zeta values. Even in the length-two case, it appears

that there are MZVs that are “irreducible” in the sense that they can’t be expressed (polynomially with rational coefficients) in terms of length one zeta values, e.g., $\zeta(6, 2)$. (Of course it isn’t known how to prove even that $\zeta(3)^2/\zeta(2)^3$ is irrational, so we have to say “appears”: but everyone since Euler who has looked for some reduction of $\zeta(6, 2)$ hasn’t found one.)

Many approaches have been used to obtain MZV identities. Analytic techniques are emphasized in the surveys [5] and [3]. In this article we will focus on algebraic techniques. It is evident that sums of form (1) constitute an algebra by simple multiplication of series: this was the starting point of [18], which formalized the “harmonic algebra” of MZVs. But, as has become fairly well known by now, there are two distinct algebra structures on the set of MZVs, the harmonic (or “shuffle”) algebra and the shuffle algebra.

Before proceeding further it is useful to introduce an algebraic notation for MZVs. Series of form (1) can be specified by the composition (finite sequence of positive integers) (i_1, i_2, \dots, i_k) ; to this composition we assign the word $x^{i_1-1}yx^{i_2-1}y \dots x^{i_k-1}y$ in noncommuting letters x and y . A series of form (1) converges exactly when $i_1 > 1$, i.e., when the corresponding word starts with x and ends with y . We call such words “admissible”, and we can think of ζ as assigning a real number to each admissible word. (It is convenient to treat the empty word 1 as admissible and set $\zeta(1) = 1$.) Note that if w is the word corresponding to a composition (i_1, \dots, i_k) , the weight $i_1 + \dots + i_k$ is the total degree $|w|$ of w . In this case the length k of the composition is the y -degree of w ; we denote this by $\ell(w)$. We will find it convenient to call $|w| - \ell(w)$ (i.e., the x -degree of w) the colength of w , denoted $c(w)$.

Let \mathfrak{H} be the underlying rational vector space of $\mathbf{Q}\langle x, y \rangle$, and let \mathfrak{H}^0 be the subspace generated by the admissible words. Then we think of ζ as a \mathbf{Q} -linear map $\zeta : \mathfrak{H}^0 \rightarrow \mathbf{R}$. Now x and y are not admissible, but \mathfrak{H}^0 is a noncommutative polynomial algebra on the words $v_{p,q} = x^p y^q$ for $p, q \geq 1$ (Of course ζ is not a homomorphism for this algebra structure). We call the length of a word $w \in \mathfrak{H}^0$ in terms of the $v_{p,q}$ its height, denoted $\text{ht}(w)$. For example, $\text{ht}(xyx^2y^2) = 2$.

With this notation, it is easy to state two identities whose proof motivated much of the early work on MZVs, the sum theorem and the duality theorem. (Both appeared in [17] as conjectures: the sum theorem was proved by Granville [13] and independently by Zagier; the duality theorem was proved via the iterated integral discussed below—see [39]—unfortunately without any notice of the conjecture!) The sum theorem can be stated as

$$\sum_{w \in \mathfrak{H}^0, |w|=n, \ell(w)=k} \zeta(w) = \zeta(n)$$

for $n \geq 2$. For the duality theorem, define an antiautomorphism τ of the noncommutative polynomial ring $\mathbf{Q}\langle x, y \rangle$ by $\tau(x) = y$ and $\tau(y) = x$; note that τ is an involution that exchanges length and colength, and preserves height. The duality theorem states that

$$\zeta(w) = \zeta(\tau(w))$$

for admissible words w .

Another of “early” results on MZVs was the Le-Murakami theorem of [25]. This is the identity

$$\sum_{w \in \mathfrak{H}^0, |w|=2n, \text{ht}(w)=k} (-1)^{\ell(w)} \zeta(w) = (-1)^n \zeta((xy)^n) \sum_{j=0}^{n-k} \binom{2n+1}{2j} (2-2j) B_{2j},$$

which they proved by examining the Kontsevich integral of the unknot.

One reason for the efficacy of the “algebraic” notation is apparent—it corresponds to the expression of MZVs by iterated integrals, as follows. Let $w = a_1 a_2 \cdots a_n$ be the factorization of an admissible word into x ’s and y ’s. Then it is easy to show that

$$\zeta(w) = \int_0^1 \int_0^{t_n} \cdots \int_0^{t_2} \frac{dt_1}{A_n(t_1)} \cdots \frac{dt_{n-1}}{A_2(t_{n-1})} \frac{dt_n}{A_1(t_n)}, \quad (2)$$

where

$$A_i(t) = \begin{cases} t, & \text{if } a_i = x, \\ 1-t, & \text{if } a_i = y. \end{cases}$$

The duality theorem follows immediately from the change of variable $(t_1, \dots, t_n) \rightarrow (1-t_n, \dots, 1-t_1)$ in the iterated integral. In addition, the fact that iterated integrals multiply via shuffle product (see the Section 2 below) implies the existence of the shuffle product structure on the set of MZVs.

But the series multiplication (or “stuffle product”) can also be formatted in terms of the algebraic notation; this is the “harmonic algebra” of [18]. The formulation in [18] led to the discovery that the harmonic algebra of MZVs is a subalgebra of the quasi-symmetric functions. We discuss this in detail in Section 3.

Another remarkable success for the algebraic method is the result of [17] that I have since (see [21]) called the derivation theorem. Let D be the derivation of $\mathbf{Q}\langle x, y \rangle$ with $D(x) = 0$ and $D(y) = xy$. Then D takes \mathfrak{H}^0 to itself, as does the derivation $\tau D \tau$. We can state the derivation theorem as

$$\zeta(D(w)) = \zeta(D(\tau(w)))$$

for admissible words w . The proof of this in [17] is an elementary but messy partial-fractions argument. It seems to have nothing to do with iterated integrals, but the algebraic notation is working some magic here—just compare the formulation above with the one given as Theorem 5.1 of [17]: for any admissible composition (i_1, \dots, i_k) ,

$$\sum_{j=1}^k \zeta(i_1, \dots, i_j + 1, \dots, i_k) = \sum_{\substack{1 \leq j \leq k \\ i_j \geq 2}} \sum_{p=0}^{i_j-2} \zeta(i_1, \dots, i_{j-1}, i_j - p, p + 1, i_{j+1}, \dots, i_k).$$

The sum, duality, and derivation theorems are all subsumed in a remarkable identity proved in 1999 by Ohno [29]. It can be stated nicely in the algebraic notation, but to do so will require some more machinery: see Section 4 below. More recently, I conjectured, and

Ohno proved, a somewhat mysterious “cyclic” analogue of the derivation theorem [21]. As with the derivation theorem, the statement in the algebraic notation is very simple, but the proof is a tricky partial-fractions argument. We discuss this in Section 5.

The “magic” of the algebraic notation seems to extend to the finite partial sums of the MZVs. Here the harmonic algebra still applies, although the shuffle algebra does not. In Section 6 we state some results on finite multiple sums, including some mod p results (p a prime). The main result of this section appears to be new.

2 The Shuffle Algebra

As above, let \mathfrak{H} be the underlying graded rational vector space of $\mathbf{Q}\langle x, y \rangle$, with x and y both given degree 1. We define a multiplication \sqcup on \mathfrak{H} by requiring that it distribute over the addition, and that it satisfy the following axioms:

- S1. For any word w , $1 \sqcup w = w \sqcup 1 = w$;
- S2. For any words w_1, w_2 and $a, b \in \{x, y\}$,

$$aw_1 \sqcup bw_2 = a(w_1 \sqcup bw_2) + b(aw_1 \sqcup w_2).$$

Induction on total degree then establishes the following.

Theorem 2.1. *The \sqcup -product is commutative and associative.*

Recall from the previous section that τ is the anti-automorphism of $\mathbf{Q}\langle x, y \rangle$ the exchanges x and y . Then we have the following fact.

Theorem 2.2. *τ is an automorphism of (\mathfrak{H}, \sqcup) .*

Proof. Since evidently $\tau^2 = \text{id}$, it suffices to show that τ is a \sqcup -homomorphism. Using the axioms S1, S2 above and induction on $|w_1 w_2|$, it is straightforward to prove that

$$w_1 a \sqcup w_2 b = (w_1 \sqcup w_2 b) a + (w_1 a \sqcup w_2) b$$

for any words w_1, w_2 and letters a, b . Now suppose inductively that $\tau(w_1 \sqcup w_2) = \tau(w_1) \sqcup \tau(w_2)$ for $|w_1 w_2| < n$, and let w_1, w_2 be words with $|w_1 w_2| = n$. We can assume both w_1 and w_2 are nonempty; write $w_1 = w'_1 a$ and $w_2 = w'_2 b$. Then

$$\begin{aligned} \tau(w_1 \sqcup w_2) &= \tau((w'_1 \sqcup w_2) a + (w_1 \sqcup w'_2) b) \\ &= \tau(a) \tau(w'_1 \sqcup w_2) + \tau(b) \tau(w_1 \sqcup w'_2) \\ &= \tau(a) (\tau(w'_1) \sqcup \tau(w_2)) + \tau(b) (\tau(w_1) \sqcup \tau(w'_2)) \\ &= \tau(a) \tau(w'_1) \sqcup \tau(b) \tau(w'_2) \\ &= \tau(w_1) \sqcup \tau(w_2). \end{aligned}$$

□

Now order the words of \mathfrak{H} as follows. For any words w_1, w_2, w_3 , set $w_1xw_2 < w_1yw_3$; and if u, v are words with v nonempty, set $u < uv$. A nonempty word w is called Lyndon if it is smaller than any of its nontrivial right factors; i.e., $w < v$ whenever $w = uv$ and $u \neq 1 \neq v$. From [31] we have the following result.

Theorem 2.3. *As a commutative algebra, (\mathfrak{H}, \sqcup) is freely generated by the Lyndon words.*

The link between the shuffle algebra and MZVs is given by the iterated integral representation (2), together with the well-known fact [32] that iterated integrals multiply by shuffle product. We can state this as follows.

Theorem 2.4. *The map $\zeta : (\mathfrak{H}^0, \sqcup) \rightarrow \mathbf{R}$ is a τ -equivariant homomorphism.*

The shuffle-product structure has been used to prove some MZV identities. For example, in [2] it is first established that

$$\sum_{r=-n}^n (-1)^r [(xy)^{n-r} \sqcup (xy)^{n+r}] = 4^n (x^2y^2)^n$$

in \mathfrak{H} , and then ζ is applied to get

$$\sum_{r=-n}^n (-1)^r \zeta((xy)^{n-r}) \zeta((xy)^{n+r}) = 4^n \zeta((x^2y^2)^n).$$

Using the known result

$$\zeta((xy)^k) = \frac{\pi^{2k}}{(2k+1)!} \quad (3)$$

(for which see the remarks following Theorem 3.5 below), together with some arithmetic, one then obtains the result conjectured by Zagier [39] several years earlier:

$$\zeta((x^2y^2)^n) = \frac{1}{2n+1} \zeta((xy)^{2n}).$$

Other shuffle convolutions are used to prove some instances of the “cyclic insertion conjecture” for MZVs in the same paper, and the topic has been revisited in [6].

3 The Harmonic Algebra and Quasi-Symmetric Functions

We can define another commutative multiplication $*$ on \mathfrak{H} by requiring that it distribute over the addition and that it satisfy the following axioms:

H1. For any word w , $1 * w = w * 1 = w$;

H2. For any word w and integer $n \geq 1$,

$$x^n * w = w * x^n = wx^n;$$

H3. For any words w_1, w_2 and integers $p, q \geq 0$,

$$x^p y w_1 * x^q y w_2 = x^p y (w_1 * x^q y w_2) + x^q y (x^p y w_1 * w_2) + x^{p+q+1} y (w_1 * w_2).$$

Note that axiom (H3) allows the $*$ -product of any pair of words to be computed recursively, since each $*$ -product on the right has fewer factors of y than the $*$ -product on the left-hand side. Induction on y -degree establishes the counterpart of Theorem 2.1.

Theorem 3.1. *The $*$ -product is commutative and associative.*

We refer to \mathfrak{H} together with its commutative multiplication $*$ as the harmonic algebra $(\mathfrak{H}, *)$. Evidently τ is *not* an automorphism of $(\mathfrak{H}, *)$. But we do have counterparts of Theorems 2.3 and 2.4, which are proved in [18].

Theorem 3.2. *As a commutative algebra, $(\mathfrak{H}, *)$ is freely generated by the Lyndon words.*

Theorem 3.3. *$(\mathfrak{H}^0, *)$ is a subalgebra of $(\mathfrak{H}, *)$, and $\zeta : (\mathfrak{H}^0, *) \rightarrow \mathbf{R}$ is a homomorphism.*

Because the multiplications $*$ and \sqcup are quite different, Theorems 2.4 and 3.3 imply that ζ has a large kernel. For example, since

$$\begin{aligned} xy * xy &= 2(xy)^2 + x^3 y \\ xy \sqcup xy &= 2(xy)^2 + 4x^2 y^2 \end{aligned}$$

we must have

$$\zeta(x^3 y - 4x^2 y^2) = 0.$$

In fact, it has been conjectured that all identities of MZVs come from comparing the two multiplications. The derivation theorem can be recovered, since

$$y \sqcup w - y * w = \tau D\tau(w) - D(w)$$

for $w \in \mathfrak{H}^0$ (Theorem 4.3 of [21]). Zudilin [41] states the conjecture as

$$\ker \zeta = \{u \sqcup v - u * v \mid u \in \mathfrak{H}^1, v \in \mathfrak{H}^0\};$$

for other formulations see [16] and [38].

Let \mathfrak{H}^1 be the vector subspace $\mathbf{Q}1 + \mathfrak{H}y$ of \mathfrak{H} ; it is evidently a subalgebra of $(\mathfrak{H}, *)$. In fact, since x is the only Lyndon word ending in x , it is easy to see that \mathfrak{H}^1 is the subalgebra of $(\mathfrak{H}, *)$ generated by the Lyndon words other than x . Note that any word $w \in \mathfrak{H}^1$ can be written in terms of the elements $z_i = x^{i-1}y$, and that the y -degree $\ell(w)$ is the length of w when expressed this way. We can rewrite the inductive rule (H3) for the $*$ -product as

$$z_p w_1 * z_q w_2 = z_p (w_1 * z_q w_2) + z_q (z_p w_1 * w_2) + z_{p+q} (w_1 * w_2). \quad (4)$$

Now for each positive integer n , define a map $\phi_n : \mathfrak{H}^1 \rightarrow \mathbf{Q}[t_1, \dots, t_n]$ (where $|t_i| = 1$ for all i) as follows. Let $\phi_n(1) = 1$ and

$$\phi_n(z_{i_1} z_{i_2} \cdots z_{i_k}) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} t_{n_1}^{i_1} t_{n_2}^{i_2} \cdots t_{n_k}^{i_k}$$

for words of length $k \leq n$, and let $\phi(w) = 0$ for words of length greater than n ; extend ϕ_n linearly to \mathfrak{H}^1 . Because the rule (4) corresponds to multiplication of series, ϕ_n is a homomorphism, and ϕ_n is evidently injective through degree n . For each $m \geq n$, there is a restriction map

$$\rho_{m,n} : \mathbf{Q}[t_1, \dots, t_m] \rightarrow \mathbf{Q}[t_1, \dots, t_n]$$

such that

$$\rho(t_i) = \begin{cases} t_i, & i \leq n \\ 0, & i > n. \end{cases}$$

The inverse limit

$$\mathfrak{P} = \text{proj} \lim_n \mathbf{Q}[t_1, \dots, t_n]$$

is the subalgebra of $\mathbf{Q}[[t_1, t_2, \dots]]$ consisting of those formal power series of bounded degree. Since the maps ϕ_n commute with the restriction maps, they define a homomorphism $\phi : \mathfrak{H}^1 \rightarrow \mathfrak{P}$.

Inside \mathfrak{P} is the algebra of symmetric functions

$$\text{Sym} = \text{proj} \lim_n \mathbf{Q}[t_1, \dots, t_n]^{\Sigma_n}$$

and also the algebra of quasi-symmetric functions (first described in [12]). We can define the algebra QSym of quasi-symmetric functions as follows. A formal series $p \in \mathfrak{P}$ is in QSym if the coefficient of $t_{i_1}^{p_1} \cdots t_{i_k}^{p_k}$ in p is the same as the coefficient of $t_{j_1}^{p_1} \cdots t_{j_k}^{p_k}$ in p whenever $i_1 < i_2 < \cdots < i_k$ and $j_1 < j_2 < \cdots < j_k$. Evidently $\text{Sym} \subset \text{QSym}$. A vector space basis for QSym is given by the monomial quasi-symmetric functions

$$M_{(p_1, p_2, \dots, p_k)} = \sum_{i_1 < i_2 < \cdots < i_k} t_{i_1}^{p_1} t_{i_2}^{p_2} \cdots t_{i_k}^{p_k},$$

which are indexed by compositions (p_1, \dots, p_k) . Since evidently $\phi(z_{i_1} \cdots z_{i_k}) = M_{(i_k, \dots, i_1)}$, we have the following result.

Theorem 3.4. *ϕ is an isomorphism of \mathfrak{H}^1 onto QSym.*

As is well known, the algebra Sym of symmetric functions is generated by the elementary symmetric functions e_i , as well as by the power-sum symmetric functions p_i (Note that we are working over \mathbf{Q}). It is easy to see that $\phi^{-1}(e_i) = z_1^i$ and $\phi^{-1}(p_i) = z_i$. Let Sym^0 be the subalgebra of the symmetric functions generated by the power-sum symmetric functions p_i with $i \geq 2$. Then $\phi^{-1}(\text{Sym}) \cap \mathfrak{H}^0 = \phi^{-1}(\text{Sym}^0)$. Since ϕ is a homomorphism, we have the following result.

Theorem 3.5. *If $a \in \phi^{-1}(\text{Sym}^0)$, then $\zeta(a)$ is a sum of products of values of $\zeta(i)$ of the zeta function with $i \geq 2$.*

In fact, the problem of expressing MZVs $\zeta(a)$ with $a \in \phi^{-1}(\text{Sym}^0)$ in terms of values of the zeta function is entirely equivalent to writing particular monomial symmetric functions in terms of power-sum symmetric functions p_i , for which there are well-known algorithms [26]. This includes cases like

$$\zeta(z_i^k) = \zeta(i, i, \dots, i)$$

(Note $i = 2$ occurs in equation (3) above), treated by analytical methods in [1]. For example, since $M_{22} = \frac{1}{2}(p_2^2 - p_4)$ in Sym^0 , we have

$$\zeta(2, 2) = \frac{1}{2}(\zeta(2)^2 - \zeta(4)) = \frac{1}{2} \left(\frac{\pi^4}{36} - \frac{\pi^4}{90} \right) = \frac{\pi^4}{120}.$$

(For a general proof of equation (3) by this method, see Corollary 2.3 of [17].)

Since y is the only Lyndon word that begins with y , we can write $\mathfrak{H}^1 = \mathfrak{H}^0[y]$ (for either the \sqcup or the $*$ product). So we can extend ζ to a map $\hat{\zeta} : \mathfrak{H}^1 \rightarrow \mathbf{R}$ by defining $\hat{\zeta}(y)$. Since

$$y * y = 2y^2 + xy \quad \text{and} \quad y \sqcup y = 2y^2,$$

there is no way to do this consistently for both multiplications, but if we restrict our attention to the $*$ -multiplication it turns out that $\hat{\zeta}(y) = \gamma$ (Euler's constant) is a happy choice. If

$$H(t) = 1 + yt + (y^2 + xy)t^2 + (y^3 + yxy + xy^2 + x^2y)t^3 + \dots$$

is the generating function for the complete symmetric functions, then the following result is easy to show (see [18]).

Theorem 3.6. $\hat{\zeta}(H(t)) = \Gamma(1 - t)$.

Now one can show (e.g., using differential equations) that

$$\sum_{w \in \mathfrak{H}^0, \text{ht}(w)=1} \zeta(w) u^{c(w)} v^{\ell(w)} = 1 - \frac{\Gamma(1-u)\Gamma(1-v)}{\Gamma(1-u-v)}.$$

Putting this together with Theorem 3.6, we have

$$\sum_{w \in \mathfrak{H}^0, \text{ht}(w)=1} \zeta(w) u^{c(w)} v^{\ell(w)} = \zeta \left(1 - \frac{H(u)H(v)}{H(u+v)} \right). \quad (5)$$

Hence $\zeta(w) \in \zeta(\phi^{-1}(\text{Sym}^0))$ for any word w of height 1 (i.e., of the form $x^p y^q$), and thus can be written in terms of ordinary zeta values $\zeta(n) = \zeta(z_n)$.

Remarkably, Ohno and Zagier [30] have recently proved that equation (5) is just the constant term of the following result.

Theorem 3.7.

$$\sum_{w \in \mathfrak{H}^0} \zeta(w) u^{c(w)} v^{\ell(w)} z^{\text{ht}(w)-1} = \frac{1}{1-z} \zeta \left(1 - \frac{H(u)H(v)}{H(\alpha)H(\beta)} \right),$$

where

$$\begin{aligned} \alpha &= \frac{1}{2} \left((u+v) + \sqrt{(u+v)^2 - 4uvz} \right) \\ \beta &= \frac{1}{2} \left((u+v) - \sqrt{(u+v)^2 - 4uvz} \right). \end{aligned}$$

The theorem implies that any sum of MZVs of fixed weight, length, and height, e.g.,

$$\sum_{|w|=6, \text{ht}(w)=2, \ell(w)=3} \zeta(w) = \zeta(3, 2, 1) + \zeta(2, 3, 1) + \zeta(2, 1, 3) + \zeta(3, 1, 2)$$

is in $\zeta(\phi^{-1}(\text{Sym}^0))$ and hence expressible in terms of $\zeta(n)$'s. But the theorem implies much more. For example, taking the limit as $z \rightarrow 1$ gives the sum theorem, and setting $v = -u$ gives the Le-Murakami theorem.

For another application of Theorem 3.6 see [20].

4 Derivations and an Action by Quasi-Symmetric Functions

As mentioned in the introduction, the derivation theorem has a far-reaching generalization proved by Ohno [29]. In this section we give a succinct statement of Ohno's theorem and some of its equivalents using the Hopf algebra structure of QSym.

We begin by motivating the use of a Hopf algebra structure in this context. (The standard references on Hopf algebras are [34] and [27], but the reader may find a source like [23] more convenient.) Let \mathcal{O} be an algebra of operators (with composition as multiplication) acting on an algebra \mathcal{A} . Then elements of the tensor product $\mathcal{O} \otimes \mathcal{O}$ act naturally on products pq for $p, q \in \mathcal{A}$: $\alpha \otimes \beta(pq) = \alpha(p)\beta(q)$. To say that $\alpha \in \mathcal{O}$ is a derivation is to say that the action of α on a products agrees with the action of $\alpha \otimes 1 + 1 \otimes \alpha$:

$$\alpha(pq) = \alpha(p)q + p\alpha(q) = (\alpha \otimes 1 + 1 \otimes \alpha)(pq).$$

A Hopf algebra structure on \mathcal{O} is essentially a “coproduct” $\Delta : \mathcal{O} \rightarrow \mathcal{O} \otimes \mathcal{O}$ compatible with the multiplication in \mathcal{O} . We require that $\alpha(pq) = \Delta(\alpha)(pq)$ for all $\alpha \in \mathcal{O}$. Elements α with $\Delta(\alpha) = \alpha \otimes 1 + 1 \otimes \alpha$ are called primitive, so the primitives in \mathcal{O} are exactly those that act as derivations. The “fine print” of the definition of a (graded connected) Hopf algebra requires that $\Delta(\alpha)$ always contain the terms $\alpha \otimes 1$ and $1 \otimes \alpha$ for α of positive degree, so primitive elements are those whose coproducts are as simple as possible. We

can generalize the notion of derivation by allowing extra terms in the coproduct. For example, a set $\{\alpha_0 = 1, \alpha_1, \alpha_2, \dots\}$ of elements is called a set of divided powers if

$$\Delta(\alpha_n) = \sum_{i+j=n} \alpha_i \otimes \alpha_j;$$

if we think of the α_n as operators, they are sometimes called a “higher derivation”. Thus, a Hopf algebra of operators is a natural extension of the notion of a Lie algebra acting by derivations.

Now $(\mathfrak{H}^1, *) \cong \mathbf{QSym}$ has a Hopf algebra structure with coproduct Δ defined by

$$\Delta(z_{i_1} z_{i_2} \cdots z_{i_n}) = \sum_{j=0}^n z_{i_1} \cdots z_{i_j} \otimes z_{i_{j+1}} \cdots z_{i_n},$$

(and counit ϵ with $\epsilon(u) = 0$ for all elements u of positive degree). This extends the well-known Hopf algebra structure on the algebra \mathbf{Sym} (as described in [10]), in which the elementary symmetric functions e_i ($\leftrightarrow y^i$) and complete symmetric functions h_i are divided powers, while the power sums p_i ($\leftrightarrow z_i$) are primitive. The Hopf algebra $(\mathfrak{H}^1, *, \Delta)$ is commutative but not cocommutative. Its (graded) dual is the Hopf algebra of noncommutative symmetric functions as defined in [11].

Now define $\cdot : \mathfrak{H}^1 \otimes \mathbf{Q}\langle x, y \rangle \rightarrow \mathbf{Q}\langle x, y \rangle$ by setting $1 \cdot w = w$ for all words w ,

$$z_k \cdot 1 = 0, \quad z_k \cdot x = 0, \quad z_k \cdot y = x^k y$$

for all $k \geq 1$, and

$$u \cdot w_1 w_2 = \sum_u (u' \cdot w_1)(u'' \cdot w_2) \tag{6}$$

where $\Delta(u) = \sum_u u' \otimes u''$; the coassociativity of Δ insures this is well-defined. It turns out (Lemma 5.2 of [21]) that $u \cdot w$ just consists of those terms of $u * w$ having the same y -degree as w , so it follows (from the associativity of $*$) that \cdot is really an action, i.e., $u \cdot (v \cdot w) = (u * v) \cdot w$. Also, equation (6) says the action makes $\mathbf{Q}\langle x, y \rangle$ a \mathbf{QSym} -module algebra, in the terminology of [23].

We note that the action of z_1 on $\mathbf{Q}\langle x, y \rangle$ is just the derivation D defined in the introduction, since $z_1 \cdot x = 0$ and $z_1 \cdot y = xy$. In fact, for each $n \geq 1$ we have a derivation D_n given by $D_n(w) = z_n \cdot w$, since the z_n are primitive in \mathbf{QSym} .

In terms of this action, we can now state Ohno’s theorem [29] as follows.

Theorem 4.1. *For any word $w \in \mathfrak{H}^0$ and nonnegative integer i ,*

$$\zeta(h_i \cdot w) = \zeta(h_i \cdot \tau(w)).$$

Recall that the h_n are divided powers, i.e., $\Delta(h_n) = \sum_{i+j=n} h_i \otimes h_j$. Only $h_1 = z_1$ is primitive, in which case we recover the derivation theorem. Taking $h_0 = 1$ gives the duality theorem, and with a little manipulation the sum theorem can also be obtained.

M. Kaneko sought to generalize the derivation theorem in another way. One can formulate the derivation theorem as saying that $(\tau D \tau - D)(w) \in \ker \zeta$ for all $w \in \mathfrak{H}^0$. Are there derivations of higher degree for which this is still true? Kaneko defined a degree- n derivation ∂_n of $\mathbf{Q}\langle x, y \rangle$ by

$$\partial_n(x) = -\partial_n(y) = x(x+y)^{n-1}y,$$

and conjectured that $\partial_n(w) \in \ker \zeta$ for all $w \in \mathfrak{H}^0$. Note $\partial_1 = \tau D \tau - D$, so the conjecture holds for $n = 1$; and the case $n = 2$ follows easily from Theorem 4.1.

Eventually Kaneko and K. Ihara proved the conjecture [22] by showing it equivalent to Theorem 4.1. One way to see this involves the action we have just defined. Extend the action of QSym on \mathfrak{H} to an action of $\text{QSym}[[t]]$ on $\mathfrak{H}[[t]]$ in the obvious way, and (as in the previous section) let

$$H(t) = 1 + h_1 t + h_2 t^2 + \cdots \in \text{QSym}[[t]]$$

be the generating function of the complete symmetric functions. If we set $\sigma_t(u) = H(t) \cdot u$ for $u \in \mathfrak{H}$, then Theorem 4.1 is equivalent to $\zeta(\bar{\sigma}_t(u) - \sigma_t(u)) = 0$ for $u \in \mathfrak{H}$, where $\bar{\sigma}_t = \tau \sigma_t \tau$. Now σ_t is an automorphism of $\mathfrak{H}^0[[t]]$: in fact $\sigma_t^{-1}(u) = E(-t) \cdot u$, where

$$E(t) = 1 + yt + y^2 t + \cdots \in \text{QSym}[[t]]$$

is the generating function of the elementary symmetric functions. Thus, Theorem 4.1 is equivalent to

$$\bar{\sigma}_t \sigma_t^{-1}(u) - u \in \ker \zeta$$

for all $u \in \mathfrak{H}^0[[t]]$. Then following result implies Kaneko's conjecture.

Theorem 4.2.

$$\bar{\sigma}_t \sigma_t^{-1} = \exp \left(\sum_{n=1}^{\infty} \frac{t^n}{n} \partial_n \right).$$

This result can be proved by showing both sides are automorphisms of $\mathfrak{H}[[t]]$ that fix t and $x + y$, and take x to $x(1 - ty)^{-1}$ (see [21]). The derivations ∂_n are related to the derivations D_n mentioned above as follows. Since

$$\frac{d}{dt} \log H(t) = \frac{H'(t)}{H(t)} = \sum_{n=1}^{\infty} p_n t^{n-1},$$

the map σ_t can also be written

$$\sigma_t = \exp \left(\sum_{n=1}^{\infty} \frac{t^n}{n} D_n \right).$$

Hence Theorem 4.2 says that

$$\exp \left(\sum_{n=1}^{\infty} \frac{t^n}{n} \partial_n \right) = \exp \left(\sum_{n=1}^{\infty} \frac{t^n}{n} \bar{D}_n \right) \exp \left(- \sum_{n=1}^{\infty} \frac{t^n}{n} D_n \right),$$

where $\bar{D}_n = \tau D_n \tau$. Thus, the ∂_n can be written in terms of the D_n and \bar{D}_n via the Campbell-Hausdorff formula. For example,

$$\partial_2 = \bar{D}_2 - D_2 - [\bar{D}_1, D_1],$$

and

$$\partial_3 = \bar{D}_3 - D_3 - \frac{3}{4}[\bar{D}_1, D_2] - \frac{3}{4}[\bar{D}_2, D_1] + \frac{1}{4}[[\bar{D}_1, D_1], D_1] - \frac{1}{4}[\bar{D}_1, [\bar{D}_1, D_1]].$$

5 Cyclic Derivations

There is an analogue of the derivation theorem involving a “cyclic derivation” $C : \mathfrak{H} \rightarrow \mathfrak{H}$. We can define C as the composition $\tilde{\mu}\hat{C}$, where $\hat{C} : \mathfrak{H} \rightarrow \mathfrak{H} \otimes \mathfrak{H}$ is the derivation sending x to 0 and y to $y \otimes x$, and $\tilde{\mu}(a \otimes b) = ba$. Here we regard $\mathfrak{H} \otimes \mathfrak{H}$ as a two-sided module over \mathfrak{H} via $a(b \otimes c) = ab \otimes c$ and $(a \otimes b)c = a \otimes bc$. Thus, e.g.,

$$\begin{aligned} C(x^3 y x y) &= \tilde{\mu}(x^3(y \otimes x)xy + x^3 y x(y \otimes x)) \\ &= \tilde{\mu}(x^3 y \otimes x^2 y + x^3 y x y \otimes x) \\ &= x^2 y x^3 y + x^4 y x y. \end{aligned}$$

This particular definition follows D. Voiculescu’s version of the cyclic derivative [37]: cyclic derivatives were first studied by Rota, Sagan and Stein [33].

In terms of the composition notation, C differs from D in that the entries are permuted cyclically, e.g.,

$$D(4, 2) = (5, 2) + (4, 3) \quad \text{versus} \quad C(4, 2) = (5, 2) + (3, 4).$$

The following result was conjectured by myself and proved by Ohno [21].

Theorem 5.1. *For any word $w \in \mathfrak{H}^1$ that is not a power of y ,*

$$\zeta(C(w)) = \zeta(\tau C \tau(w)).$$

As mentioned in the introduction, the proof uses partial fractions.

The difference between C and D is most striking when applied to periodic words. For example, Theorem 5.1 applied to $w = (x^2 y)^n$ gives (in the composition notation)

$$\zeta(4, 3, \dots, 3) = \zeta(3, 3, \dots, 3, 1) + \zeta(2, 3, \dots, 3, 2).$$

Theorem 5.1 also gives a very nice proof of the sum theorem. Here is the idea: Let $u = x + ty$. Then the coefficient of t^k in $xu^{n-2}y$ is the sum of all words $w \in \mathfrak{H}^0$ with $|w| = n$ and $\ell(w) = k$. Now

$$C(u^{n-1}) = (n-1)txu^{n-2}y \quad \text{while} \quad \tau C \tau(u^{n-1}) = (n-1)xu^{n-2}y,$$

so the cyclic derivation theorem implies that ζ applied to the coefficient of t^{k-1} equals ζ applied to the coefficient of t^k . That is, the sum of MZVs of fixed weight n and length k must be independent of k (and so must be $\zeta(n)$).

Here is another corollary of Theorem 5.1, stated in terms of the action of QSym on $\mathbf{Q}\langle x, y \rangle$.

Theorem 5.2. For $m, n \geq 1$, $\zeta(z_n \cdot xy^m) = \zeta(z_m \cdot xy^n)$.

Just as the derivation theorem extends to Theorem 4.1, it is natural to ask if the cyclic derivation theorem can be extended. It is easy to define cyclic derivations C_n analogous to the D_n of the last section: just set $C_n = \tilde{\mu}\hat{C}_n$, where $\hat{C}_n(x) = 0$ and $\hat{C}_n(y) = y \otimes x^n$. One could then try to define cyclic derivations analogous to Kaneko's derivations ∂_n (which are expressible in terms of commutators of the D_n and \bar{D}_n). The difficulty appears to be in defining the commutator of cyclic derivations.

6 Finite Multiple Sums and Mod p Results

In this section we consider the finite sums

$$A_{(i_1, \dots, i_k)}(n) = \sum_{n \geq n_1 > n_2 > \dots > n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}}$$

and

$$S_{(i_1, \dots, i_k)}(n) = \sum_{n \geq n_1 \geq n_2 \geq \dots \geq n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}}$$

where the notation is patterned after that of [17]; the multiple zeta values of the previous sections are

$$\zeta(i_1, \dots, i_k) = \lim_{n \rightarrow \infty} A_{(i_1, \dots, i_k)}(n),$$

when the limit exists (i.e., when $i_1 > 1$).

The sums $A_I(n)$ and $S_I(n)$ are related in an obvious way, e.g.,

$$S_{(4,2,1)}(n) = A_{(4,2,1)}(n) + A_{(6,1)}(n) + A_{(4,3)}(n) + A_{(7)}(n).$$

We can formalize the relation as follows. For compositions I, J , we say I refines J (denoted $I \succ J$) if J can be obtained from I by combining some of its parts. Then

$$S_I(n) = \sum_{I \succeq J} A_J(n). \tag{7}$$

Of course $S_{(m)}(n) = A_{(m)}(n)$ for all m, n .

It will be useful to have some additional notations for compositions. We adapt the notation used in previous sections for words, so for $I = (i_1, \dots, i_k)$ the weight of I is $|I| = i_1 + \dots + i_k$, and $k = \ell(I)$ is the length of I . For $I = (i_1, \dots, i_k)$, the reversed composition (i_k, \dots, i_1) will be denoted \bar{I} : of course reversal preserves weight, length and refinement (i.e., $I \succeq J$ implies $\bar{I} \succeq \bar{J}$).

Compositions of weight n are in 1-to-1 correspondence with subsets of $\{1, 2, \dots, n-1\}$ via partial sums

$$(i_1, i_2, \dots, i_k) \rightarrow \{i_1, i_1 + i_2, \dots, i_1 + \dots + i_{k-1}\},$$

and $I \preceq J$ if and only if the subset corresponding to I contains that corresponding to J . Complementation in the power set then gives rise to an involution $I \rightarrow I^*$; e.g., $(1, 1, 2)^* = (3, 1)$. Evidently $|I^*| = |I|$ and $\ell(I) + \ell(I^*) = |I| + 1$. Also, $I \preceq J$ if and only if $I^* \succeq J^*$. Finally, for two compositions I and J we write $I \sqcup J$ for their juxtaposition.

From [17] we have formulas for symmetric sums of $A_I(n)$ and $S_I(n)$ in terms of length one sums $S_{(m)}(n)$. (Though the proofs in [17] are given for infinite series, they carry over to the finite case.) They require some notation to state. For a partition $\Pi = \{P_1, \dots, P_l\}$ of the set $\{1, 2, \dots, k\}$, let

$$c(\Pi) = \prod_{s=1}^l (\text{card } P_s - 1)! \quad \text{and} \quad \tilde{c}(\Pi) = (-1)^{k-l} \prod_{s=1}^l (\text{card } P_s - 1)!,$$

and if also $I = (i_1, \dots, i_k)$ is a composition of length k , let

$$S(n, \Pi, I) = \prod_{s=1}^l S_{(p_s)}(n), \quad \text{where} \quad p_s = \sum_{j \in P_s} i_j.$$

If $I = (i_1, \dots, i_k)$ is a composition of length k , then elements $\sigma \in \Sigma_k$ of the symmetric group act on I via $\sigma \cdot I = (i_{\sigma(1)}, \dots, i_{\sigma(k)})$. Then Theorems 2.1 and 2.2 of [17] give us the following result.

Theorem 6.1. *For all positive integers k and n and compositions I of length k ,*

$$\begin{aligned} \sum_{\sigma \in \Sigma_k} S_{\sigma \cdot I}(n) &= \sum_{\text{partitions of } \{1, \dots, k\}} c(\Pi) S(n, \Pi, I) \\ \sum_{\sigma \in \Sigma_k} A_{\sigma \cdot I}(n) &= \sum_{\text{partitions of } \{1, \dots, k\}} \tilde{c}(\Pi) S(n, \Pi, I) \end{aligned}$$

Because of the correspondence between compositions and noncommutative words in \mathfrak{H}^1 , we have (for any fixed n) a map $\rho_n : \mathfrak{H}^1 \rightarrow \mathbf{Q}$ sending $w \in \mathfrak{H}^1$ to $A_{I(w)}(n)$, where $I(w)$ is the composition associated with w . Note that ρ_n is the composition $\text{ev} \circ T \circ \phi_n$, where ϕ_n is the map defined in Section 3, T is the automorphism of QSym sending M_I to $M_{\bar{I}}$, and ev is the function that sends t_i to $\frac{1}{i}$. Thus, $\rho_n : (\mathfrak{H}^1, *) \rightarrow \mathbf{R}$ is a homomorphism. We can combine the homomorphisms ρ_n into a homomorphism ρ that sends $w \in \mathfrak{H}^1$ to the real-valued sequence $n \rightarrow \rho_n(w)$. We shall write A_I for the real-valued sequence $n \rightarrow A_I(n)$ (and similarly for S_I), so ρ sends w to $A_{I(w)}$.

Now QSym has various integral bases besides the M_I . In the literature one often sees the fundamental quasi-symmetric functions

$$F_I = \sum_{J \succeq I} M_J,$$

but we will be concerned with what we call the “essential” quasi-symmetric functions

$$E_I = \sum_{J \preceq I} M_J.$$

In view of equation (7), the homomorphism ρ_n sends E_I to $S_I(n)$.

Since \mathbf{QSym} is a commutative Hopf algebra, its antipode S is an automorphism of \mathbf{QSym} and $S^2 = \text{id}$. Now S can be given by the following explicit formulas: for proof see [7] or [19].

Theorem 6.2. *The antipode S of \mathbf{QSym} is given by*

1. $S(M_I) = \sum_{I_1 \sqcup I_2 \sqcup \dots \sqcup I_l = I} (-1)^l M_{I_1} M_{I_2} \cdots M_{I_l};$
2. $S(M_I) = (-1)^{\ell(I)} E_{\bar{I}}.$

Part (2) of this result says that the E_I have essentially the same multiplication rules as the M_I : if T is the automorphism of \mathbf{QSym} defined above, then $S \circ T$ takes any identity among the M_I to an identity among the E_I that differs only in signs. For example, since

$$M_{(2)}M_{(3)} = M_{(2,3)} + M_{(3,2)} + M_{(5)}$$

we have

$$E_{(2)}E_{(3)} = E_{(2,3)} + E_{(3,2)} - E_{(5)}.$$

Now define an automorphism ψ of $\mathbf{Q}\langle x, y \rangle$ by

$$\psi(x) = x + y, \quad \psi(y) = -y$$

Evidently $\psi^2 = \text{id}$, and $\psi(\mathfrak{H}^1) = \mathfrak{H}^1$. Thus ψ defines a linear involution of $\mathfrak{H}^1 \cong \mathbf{QSym}$ (which is *not*, however, a homomorphism for the $*$ -product). We can describe the action of ψ on the integral bases for \mathbf{QSym} as follows.

Theorem 6.3. *For any composition I ,*

1. $\psi(M_I) = (-1)^{\ell(I)} F_I$
2. $\psi(E_I) = -E_{I^*}$

Proof. Suppose $w = w(I)$ is the word in x and y corresponding to a composition I . Then evidently substituting y in place of any particular factor x in w corresponds to splitting a part of I . With this observation, part (1) is clear (there is also one factor of -1 for each occurrence of y in w).

Now we prove part (2). We have

$$\psi(E_I) = \sum_{J \preceq I} \psi(M_J) = \sum_{J \preceq I} (-1)^{\ell(J)} F_J$$

from part (1). From Example 1 of [19], $S(F_I) = (-1)^{|I|} F_{\bar{I}^*}$, where S is the antipode of \mathbf{QSym} . Thus

$$\begin{aligned} S\psi(E_I) &= \sum_{J \preceq I} (1)^{\ell(J)+|J|} F_{\bar{J}^*} = - \sum_{J \preceq I} (-1)^{\ell(J^*)} F_{\bar{J}^*} \\ &= - \sum_{\bar{J}^* \succeq \bar{I}^*} (-1)^{\ell(\bar{J}^*)} F_{\bar{J}^*} = - \sum_{K \succeq \bar{I}^*} (-1)^{\ell(K)} F_K. \end{aligned}$$

Now by Möbius inversion,

$$F_I = \sum_{I \preceq J} M_J \quad \text{implies} \quad M_I = \sum_{I \preceq J} (-1)^{\ell(I) - \ell(J)} F_J,$$

and so

$$S\psi(E_I) = -(-1)^{\ell(\bar{I}^*)} M_{\bar{I}^*}$$

Apply S to both sides to get

$$\psi(E_I) = -(-1)^{\ell(I^*)} (-1)^{\ell(\bar{I}^*)} E_{I^*} = -E_{I^*}.$$

□

We consider two operators on the space $\mathbf{R}^{\mathbf{N}}$ of real-valued sequences. First, there is the partial-sum operator Σ , given by

$$\Sigma a(n) = \sum_{i=0}^n a(i)$$

for $a \in \mathbf{R}^{\mathbf{N}}$. Second, there is the operator ∇ given by

$$\nabla a(n) = \sum_{i=0}^n \binom{n}{i} (-1)^i a(i).$$

It is easy to show that Σ and ∇ generate a dihedral group within the automorphisms of $\mathbf{R}^{\mathbf{N}}$, i.e., $\nabla^2 = \text{id}$ and $\Sigma\nabla = \nabla\Sigma^{-1}$. It follows that $(\Sigma\nabla)^2 = \text{id}$. We have the following result on multiple sums.

Theorem 6.4. *For any composition I , $\Sigma\nabla S_I = -S_{I^*}$.*

Proof. We proceed by induction on $|I|$. The weight one case is $\Sigma\nabla S_{(1)} = \nabla\Sigma^{-1}S_{(1)} = -S_{(1)}$, i.e.

$$\sum_{k=1}^n \frac{(-1)^k}{k} \binom{n}{k} = -\sum_{k=1}^n \frac{1}{k},$$

which is a classical (but often rediscovered) formula; it actually goes back to Euler [9]. For $I = (i_1, i_2, \dots, i_k)$, it is straightforward to show that $\nabla S_I(n) = \frac{1}{n} \nabla f(n)$, where $f \in \mathbf{R}^{\mathbf{N}}$ is given by

$$f(n) = \begin{cases} S_{(i_2, \dots, i_k)}(n), & \text{if } i_1 = 1; \\ \Sigma^{-1} S_{(i_1-1, i_2, \dots, i_k)}(n), & \text{otherwise.} \end{cases}$$

Now suppose the theorem has been proved for all I of weight less than n , and let $I = (i_1, \dots, i_k)$ have weight n . There are two cases: $i_1 = 1$, and $i_1 > 1$. In the first case, let $(i_2, \dots, i_k)^* = J = (j_1, \dots, j_r)$. By the assertion of the preceding paragraph and the induction hypothesis,

$$\Sigma\nabla S_I(n) = \Sigma\left(\frac{1}{n} \nabla S_{J^*}(n)\right) = -\Sigma\left(\frac{1}{n} \Sigma^{-1} S_J(n)\right) = -S_{(j_1+1, j_2, \dots, j_r)}(n).$$

But evidently $I^* = (j_1 + 1, j_2, \dots, j_r)$, so the theorem holds in this case

If $i_1 > 1$, we instead write $(i_1 - 1, i_2, \dots, i_k)^* = J = (j_1, \dots, j_r)$. Then

$$\Sigma \nabla S_I(n) = \Sigma \left(\frac{1}{n} \nabla \Sigma^{-1} S_{J^*}(n) \right) = \Sigma \left(\frac{1}{n} \Sigma \nabla S_{J^*}(n) \right) = -\Sigma \left(\frac{1}{n} S_J(n) \right) = -S_{(1, j_1, \dots, j_r)}(n).$$

But in this case $I^* = (1, j_1, \dots, j_r)$, so the theorem holds in this case as well. \square

The proof of the preceding result is essentially a formalization of the procedure in App. B of [36]. (For a recent occurrence of the special case $I = (1, 1, 1)$ as a problem, see [15].) Theorem 6.4, together with part (2) of Theorem 6.3, says that the diagram

$$\begin{array}{ccc} \text{QSym} & \xrightarrow{\psi} & \text{QSym} \\ \rho \downarrow & & \rho \downarrow \\ \mathbf{R}^N & \xrightarrow{\Sigma \nabla} & \mathbf{R}^N \end{array} \quad (8)$$

commutes.

For the rest of this section, we discuss mod p results about $S_I(p-1)$ and $A_I(p-1)$, where p is a prime. (Some results of this type appear in [40].) For prime p , the sums $A_I(p-1)$ and $S_I(p-1)$ contain no factors of p in the denominators, and can be regarded as elements of the field $\mathbf{Z}/p\mathbf{Z}$. The following result about length one harmonic sums is well known (cf. [14], pp. 86-88).

Theorem 6.5. $S_{(k)}(p-1) \equiv 0 \pmod{p}$ for all prime $p > k + 1$.

Because Theorem 6.1 expresses symmetric sums of $S_I(p-1)$ and $A_I(p-1)$ in terms of length one sums, any such symmetric sum is zero mod p for $p > |I| + 1$. In particular, for $I = (k, k, \dots, k)$ (r repetitions), we have

$$A_I(p-1) \equiv S_I(p-1) \equiv 0 \pmod{p}$$

for prime $p > rk + 1$ (cf. Theorem 1.5 of [40]). There is the following result relating sums associated to I and \bar{I} (cf. Lemma 3.2 of [40]).

Theorem 6.6. For any composition I , $A_I(p-1) \equiv (-1)^{|I|} A_{\bar{I}}(p-1) \pmod{p}$, and similarly $S_I(p-1) \equiv (-1)^{|I|} S_{\bar{I}}(p-1) \pmod{p}$.

Proof. Let $I = (i_1, \dots, i_k)$. Working mod p , we have

$$\begin{aligned} A_I(p-1) &\equiv \sum_{p > a_1 > \dots > a_k > 0} \frac{1}{a_1^{i_1} \dots a_k^{i_k}} \equiv \sum_{p > a_1 > \dots > a_k > 0} \frac{(-1)^{i_1 + \dots + i_k}}{(p - a_1^{i_1}) \dots (p - a_k^{i_k})} \\ &\equiv \sum_{0 < b_1 < \dots < b_k < p} \frac{(-1)^{i_1 + \dots + i_k}}{b_1^{i_1} \dots b_k^{i_k}} = (-1)^{|I|} A_{\bar{I}}(p-1), \end{aligned}$$

and similarly for S_I . \square

An immediate consequence is that $S_I(p-1) \equiv A_I(p-1) \equiv 0 \pmod p$ if $I = \bar{I}$ and $|I|$ is odd. Another consequence is that $S_{(i,j)}(p-1) \equiv A_{(i,j)}(p-1) \equiv 0 \pmod p$ when $p > i+j+1$ and $i+j$ is even. This is because

$$S_{(i,j)}(p-1) + S_{(j,i)}(p-1) \equiv 0 \pmod p$$

for $p > i+j+1$ by Theorem 6.1, while $S_{(i,j)}(p-1) \equiv S_{(j,i)}(p-1) \pmod p$ when $i+j$ is even by Theorem 6.6.

We have the following result relating S_I and S_{I^*} .

Theorem 6.7. $S_I(p-1) \equiv -S_{I^*}(p-1) \pmod p$ for all primes p .

Proof. Let f be a sequence. From the definition of ∇

$$\Sigma \nabla f(n) = \sum_{i=0}^n \binom{n+1}{i+1} (-1)^i f(i),$$

so taking $n = p-1$ gives

$$\Sigma \nabla f(p-1) \equiv (-1)^{p-1} f(p-1) \equiv f(p-1) \pmod p.$$

Now take $f = S_I$ and apply Theorem 6.4. □

This result has the following corollary for the A_I , which may be compared with Theorem 4.4 of [17]. (We use superscripts for repetition, so $(n, 1^k)$ means the composition of weight $n+k$ with k repetitions of 1.)

Theorem 6.8. *If p is a prime with $p > \max\{k+1, n\}$, then*

$$A_{(n, 1^k)}(p-1) \equiv A_{(k+1, 1^{n-1})}(p-1) \pmod p.$$

Proof. First note that $(n, 1^k)^* = (1^{n-1}, k+1)$. So, combining Theorems 6.7 and 6.6,

$$S_{(n, 1^k)}(p-1) \equiv -S_{(1^{n-1}, k+1)}(p-1) \equiv (-1)^{n+k+1} S_{(k+1, 1^{n-1})}(p-1) \pmod p. \quad (9)$$

Now equate the right-hand sides of parts (1) and (2) of Theorem 6.2 and then apply ρ_{p-1} to get

$$(-1)^{\ell(I)} S_{\bar{I}}(p-1) = \sum_{I_1 \sqcup \dots \sqcup I_l = I} (-1)^l A_{I_1}(p-1) \cdots A_{I_l}(p-1)$$

for any composition I ; if we set $I = (1^k, n)$, the hypothesis insures that all the terms on the right-hand side are zero mod p except the one with $l = 1$, giving $(-1)^k S_{(n, 1^k)}(p-1) \equiv A_{(1^k, n)}(p-1) \pmod p$. Apply Theorem 6.6 to get $S_{(n, 1^k)}(p-1) \equiv (-1)^n A_{(n, 1^k)}(p-1) \pmod p$. By the same argument, $S_{(k+1, 1^{n-1})}(p-1) \equiv (-1)^{k+1} A_{(k+1, 1^{n-1})}(p-1) \pmod p$, and equation (9) gives the conclusion. □

We can state Theorem 6.7 in algebraic language as follows. Define, for each prime p , a map $\chi_p : \mathfrak{H}_{\mathbf{Z}}^1 \rightarrow \mathbf{Z}/p\mathbf{Z}$ by $\chi_p(w) = \rho_{p-1}(w)$. (Here $\mathfrak{H}_{\mathbf{Z}}^1$ is the integral version of \mathfrak{H}^1 , i.e., the graded \mathbf{Z} -module in $\mathbf{Z}\langle x, y \rangle$ generated by words ending in y .) The commutative diagram (8) gives the following algebraic version of Theorem 6.7, which can be considered a mod p counterpart of the duality theorem for MZVs.

Theorem 6.9. *As elements of $\mathbf{Z}/p\mathbf{Z}$, $\chi_p(w) = \chi_p(\psi(w))$ for words w of \mathfrak{H}^1 .*

For example, since $\psi(x^2y^3) = -x^2y^3 - xy^4 - yxy^3 - y^5$, we have

$$A_{(3,1,1)}(p-1) \equiv -A_{(3,1,1)}(p-1) - A_{(2,1,1,1)}(p-1) - A_{(1,2,1,1)}(p-1) - A_{(1,1,1,1,1)}(p-1) \pmod{p}.$$

For $p > 6$ this reduces to $2A_{(3,1,1)}(p-1) \equiv -A_{(2,1,1,1)}(p-1) - A_{(1,2,1,1)}(p-1) \pmod{p}$.

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